Matheson gas gives N2 max impurity level for 5N Xe as <3 ppmv

$$ppmv := 10^{-6}$$

 $C_{N2_Xe} := 3 \cdot ppmv$ This is a volumetric density ratio, which is a mole ratio, not a mass ratio no ratio is given for N2 in 5N Ar, but N2 in 5N He is same value, for N2 in 5N Kr it is 10ppmv assume 5N Ar has 3ppmv N2

The Pureguard purifier claims it delivers <1ppb N2 for 30 SLPM (once through flow) for one year, this flow rate is as defined elsewhere one standard cubic cm of gas is:

$$scc = 4.464 \times 10^{-5} \text{ mol}$$
 so -->> $SLPM := 10^{3} scc \cdot min^{-1}$ $SLPM = 7.44 \times 10^{-4} mol \cdot s^{-1}$

molar gas flow rate:

$$q_{gas} := 30SLPM$$
 $q_{gas} = 0.022 \,\text{mol} \cdot \text{s}^{-1}$

at 15 bar pressure, room temp., this is a volumetric flow rate:

$$v_{gas} := q_{gas} \cdot \frac{\left(R \cdot 293K\right)}{15bar}$$
 $v_{gas} = 0.036L \cdot s^{-1}$

If we assume that we cannot increase the molar flow through the getter (high flow restiction? damage?) then we have an initial molar removal rate:

$$q_{N2t0} := C_{N2_Xe} \cdot q_{gas}$$
 $q_{N2t0} = 6.696 \times 10^{-8} \text{ mol·s}^{-1}$

this removal rate is constant for a once through gas system, so we can estimate capacity, assuming the purifier is saturated after this:

$$\begin{aligned} &Q_{N2} := q_{N2t0} \cdot 1 \text{yr} \\ &Q_{N2} = 2.113 \, \text{mol} \qquad Q_{N2} = 4.734 \times \, 10^4 \, \text{scc} \\ &M_{N2} := Q_{N2} \cdot M_{a_N} \qquad M_{N2} = 29.6 \, \text{gm} \end{aligned} \qquad M_{a_N} := 14 \, \text{gm} \cdot \text{mol}^{-1}$$

Assume we have a total quantity of Xe in vessel: density at 15 bara

$$\begin{aligned} & \text{M}_{Xe} = 147.9\,\text{kg} \quad \text{N}_{Xe} \coloneqq \text{M}_{Xe} \cdot \text{M}_{a_Xe}^{-1} \quad \text{N}_{Xe} = 1.088 \times 10^3\,\text{mol} \quad \rho_{Xe} \coloneqq .091\,\frac{\text{gm}}{\text{cm}^3} \qquad \text{V}_{Xe} \coloneqq \text{M}_{Xe} \cdot \rho_{Xe}^{-1} \\ & \text{This would have, at 5N purity} : \qquad \qquad & \text{cm}^3 \\ & \text{N}_{N2} \coloneqq \text{N}_{Xe} \cdot \text{C}_{N2} \quad \text{Xe} \qquad & \text{N}_{N2} = 3.263 \times 10^{-3}\,\text{mol} \end{aligned}$$

The similarly priced SAES getter, rated at 5 SLPM for 1 year would only get 1/6 of this, but would still have plenty of capacity for 5N Xe. Our EXe is likely more pure than 5N

Since impurity concentration removal rate will go down, as gas gets cleaner (because we cannot increase molar flow rate beyond rated value), time to reach a certain impurity level (assuming first, no outgassing of components) is

molar rate of change = molar rate of inflow - molar rate of outflow.

$$\frac{d}{dt}Q := 0 - q_{gas}$$

 $\frac{d}{dt}Q := -\frac{Q}{V} \cdot v_{gas} \qquad \text{where V is vessel volume and Q is amount of N2 in vessel, in mol}$

$$\frac{1}{Q}dQ := -\frac{v_{gas}}{V}dt$$

integrating both sides

$$\ln(Q) - \ln\!\left(Q_0\right) \coloneqq -\frac{t \cdot v_{gas}}{V} \text{ or } \qquad \ln\!\left(\frac{Q}{Q_0}\right) \coloneqq \frac{-t \cdot v_{gas}}{V} \text{ or } \qquad \qquad Q \coloneqq Q_0 \cdot e^{\frac{-t \cdot v_{gas}}{V}}$$

time to reach 1 ppb N2

$$t_{1ppb} \coloneqq \ln \left(\frac{10^{-9}}{3 \cdot 10^{-6}} \right) \cdot \frac{-V_{Xe}}{v_{gas}}$$

$$t_{1ppb} = 4.156 \, day \qquad \text{or 25 days for SAES getter}$$

Adding in outgassing from internal components and area, we will need the general form of solution for 1st order ODE. First we need to quantify an outgassing rate which will change as concentration in plastic goes down over time. However, we can see qualitatively, that impurity level in the gas may rise before it falls, if initial outgassing rate is higher than initial removal rate.

to be continued...